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A Monte Carlo Simulation of Thermal Driven Fluid: Flux Rate and Density Profile

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Abstract: Effects of uniform temperature and linear temperature gradient on flow rate and density profile of fluid driven from a source to an open system is studied by a Monte Carlo simulation in three dimensions. The steady-state density profile with uniform temperature differs significantly from that of the temperature gradient at all but high temperature regimes where the profile is a linear density gradient; the crossover to linear density gradient of the profile is sensitive to range of temperature variation. The response of the flow rate density to the temperature is nonlinear.

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Understanding the flow of methane gas below the ocean floor is of considerable interest particularly in context to geochemical and geophysical characteristics of methane hydrate in marine sediments [1-10]. At the temperatures and pressures within the marine sediments, the gas (usually Methane) is in solution. Systematic experimental observations of flow and density profile of methane gas are severely limited due to uncontrollable parameters such as changes in pressure and temperature gradients and morphological variations of the host matrix, i.e., the evolution of porous ground [5-7]. One of the major problems in modeling such a complex system is to incorporate all the details on a large scale [11]. Therefore, identifying their contributions, such as effects of temperature gradient, pressure gradient, porosity etc. on such properties as flow rate of methane and its density profile is very difficult [12,13]. Obviously, this requires long term study involving model developments and analysis of resulting data. It would be, therefore, desirable to focus on one parameter, i.e., temperature gradient, at a time and understand its role, as attempted in this paper before including other parameters in the model.

We consider a discrete lattice of size $L \times L \times L_z$. As in our earlier model, the bottom plane ($z = 0$) is connected to a source of fluid (i.e., methane in solution) modeled by an interacting lattice gas. The top plane ($z = L_z$) of the lattice is open, i.e., a gas particle can escape from top. In order to consider interaction, we introduce an interaction density (ρ_i) to each lattice site i : $\rho_i = 1$ if site i is occupied by a fluid particle and $\rho_i = -1$ if site i is empty. The interaction Hamiltonian is given by,

$$E = U \sum_{ij} \rho_i \rho_j, \quad (1)$$

where U is the interaction strength; we set $U = 1$ in unit of Boltzmann constant (k_B) but U can be varied if needed in order to incorporate specific effects such as drag/viscosity of the host matrix. The summation in eq. 1 is restricted to nearest neighbor sites. Initially, the entire lattice is empty except the first plane ($z = 1$) connected to the source which is filled with fluid, one particle at each site.

Two thermal systems are considered: (i) homogeneous temperature (T) throughout the sample from bottom to top and (ii) a linear temperature gradient,

$$T(z) = (T_b - T_t)/z, \quad (2)$$

where $T(z)$ is the temperature of z -th plane and $T_b = T(z = 1)$, $T_t = T(z = L_z)$. The temperature at the top plane $T_t = 0$ is fixed while the temperature at the bottom plane T_b is varied. Fluid particle executes its stochastic motion with the Metropolis algorithm: a particle at site i and one of its neighboring site j are chosen randomly. If site j is empty then we accept the move with the Boltzmann probability $\exp(-\Delta E/k_B T)$, where ΔE is the change in energy due to corresponding configurational changes, i.e., from $\rho_i = 1, \rho_j = -1$ to $\rho_i = -1, \rho_j = 1$. Energy and temperature are measured in arbitrary unit (normalized by the Boltzmann constant (k_B)). Periodic boundary condition is used along x - and y -directions and open condition along (z -)direction. Thus, a fluid particle can escape from the top ($z = L_z$) but cannot go below the bottom layer ($z = 1$). An attempt to move each particle once is defined as one Monte Carlo Step (MCS). As soon as a site in the bottom plane ($z = 1$) is vacated by a mobile gas particle, it is filled by a particle from the source. Note that the number of particles is not conserved.

As the simulation proceeds, the fluid flows from bottom to top and the density profile evolves. During the simulation we monitor the overall mobility of fluid particles and their center of mass, flow rate of fluid, and their density profile. The simulation is repeated for a large number of independent runs in order to estimate the average values of the steady-state flow rate and equilibrium density profile. In the steady-state, the flow rate of fluid is independent of time and the density profile becomes constant (see below). The simulation is carried out on different lattice sizes but most simulations are performed with 30^3 and 60^3 samples; we have not seen severe finite size effects on the qualitative behavior. Figure 1 shows the variation of net mass of the fluid flow, i.e., the fluid flux (ϕ) with MCS time along the vertical (z) direction. The linear derivative of mass flow with time leads to fluid current,

$$i = \frac{d\phi}{dt}, \quad (3)$$

and current density,

$$j = i/A, \quad (4)$$

where $A = L^2$, the cross-sectional area. The linear variation of the data suggests that the flow rate is independent of time. This implies that our system has reached the steady-state.

The response of the flow rate density to temperature is nonlinear (figure 2). Generally the flow rate response is low at low temperatures and high

temperatures with a large change in response rate in between. The nonlinear pattern of the response with uniform temperature is not much different from the linear temperature gradient except the range of temperatures.

The steady-state density profiles at different temperatures (case (i)) and temperature gradients (case (ii)) are presented in figure 3. We note a significant difference in the density profiles in systems with uniform temperature and linear temperature gradients. With the uniform temperature, a sigmoidal form of profile develops except at high temperatures ($T = 2.0, 3.0$) where the density decays approximately linearly from bottom to top. At low to moderate temperatures ($T = 0.0167 - 1.0$), three linear density gradients are observed: a slow linear decay from bottom in lower half of the sample ($z = 1 - 12$) is followed by a large density decay in few planes ($z = 15 - 19$) before the onset of a low linear decay toward the top. In presence of linear temperature gradient on the other hand, the approach to linear density profiles at high values of T_b ($=3.0 - 10.0$), is more step-like (see fig 3(b)); the crossover to linear decay of density in upper part of the sample is rather slow. In either case, the effect of temperature change is very important in orchestrating the shape of the density profile. Note that, in addition to temperature, the density gradient also plays a significant part in driving the fluid density from bottom to top. Thus, if the measurement of temperature profile below the ocean floor is available, i.e., uniform and/or linear gradient, then, one would be able to gain an insight into the density profile of methane in solution and possibly the location of methane hydrate formation.

Connecting such qualitative results to quantitative field measurement is one of the major problem in such simulations. Scaling and calibration of the physical quantities and variables (time steps, temperature, and lattice size) with the measured quantities are needed in order to gain insight into the applicability of these findings in the range of variables. Unfortunately, field measurements for systematic variation of the density profile or the flux rate of methane [13] with depth and temperature gradient is not available at present. Neither it is feasible to approach the relevant scale of marine geosystem in computational models from microscopic scale. Therefore, it is rather difficult to connect these results to limited field measurements in a meaningful way. However, it is worth pointing out the order of scales even with our coarse-grained approach. Typically, a temperature gradient below the ocean floor is about $20^{\circ}\text{C}/\text{km}$. Our temperature gradient $\Delta T/z \sim 20^{\circ}\text{C}/\text{km}$, leads to energy of gas of the order of $10^{-19}\text{J} \sim 1\text{ eV}$ if we scale the temperature T with

the Boltzmann constant and $z \sim 1\text{km}$. Equipartition of energy, provides an estimate of particle speed $\sim 37\text{ m/s}$. The variation in the the temperature gradients are selected to explore the changes in density profile and response of the flow rate. Now, let us look at the advance of the fluid front to estimate the time steps. A typical variation of the center of mass of the fluid with time is presented in figure 4. This gives the front velocity as 0.02 lattice constant / time steps. Since we have assume the size of the sample to be 1.0 cm, one lattice constant is 0.033 cm on a 30^3 lattice. In order to match the fluid flow rate of 1 mm/yr [13] in field measurement, our time step should be of the order of a month. However, if the field measurement for the flow rate is lower then our MC step has to be increased accordingly. Note that we do not have field measurements suitable for our idealized model and therefore, these estimates are mainly to illustrate the method.

In summary, a computer simulation model is presented to show that the density profile of fluid driven from a source into an open system depends on temperature and the temperature gradient: specific profiles are proposed for a range of temperature and temperature gradients. The flow rate density responds nonlinearly to variations in temperature and gradient. Even the simple "toy model" like this one is computationally intensive for the complex issues addressed here but provides insight into evolution of density profile and flow rate that would be encountered with methane in solution moving through marine sediments.

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Figure Captions:

Figure 1: Net mass of gas flow along z -direction versus MCS time. 60^3 sample is used with 10 independent runs at $T_b = 0.5$

Figure 2: Variation of the flow rate density of gas with temperature. Sample of size 30^3 is used with up to 50 independent runs.

Figure 3: Density profile for uniform temperature (T) (a) and linear temperature gradient (b) with various T and T_b ; samples of size 30^3 is used with 20-50 independent runs.

Figure 4: Variation of the center of mass of the gas with time step on a 30^3 lattice for three temperature gradients. Statistics is the same as in figure 3. The dotted lines are the least square fit and give a slope of about 0.02.

Figure 1

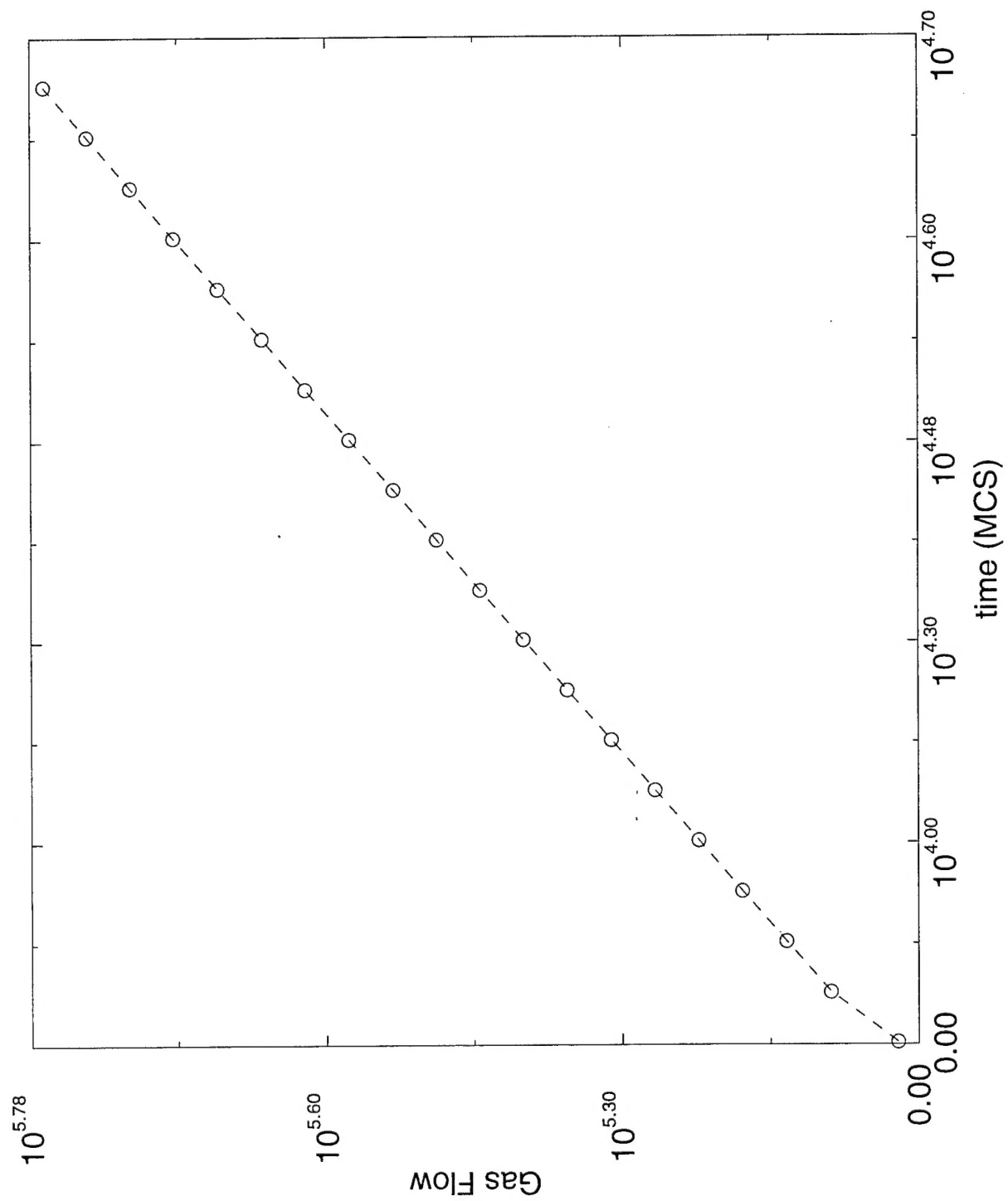


Figure 2

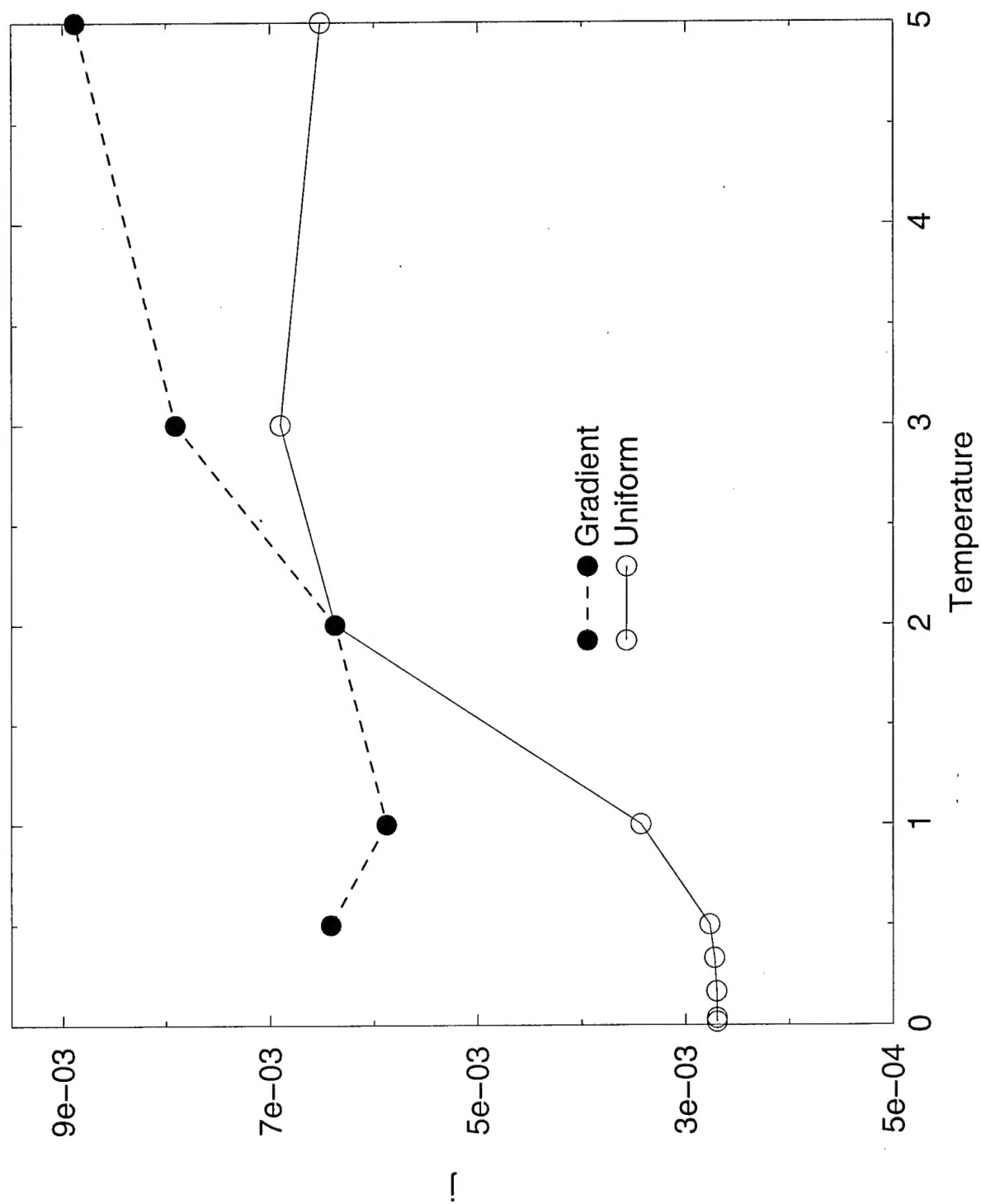


Figure 3(a)

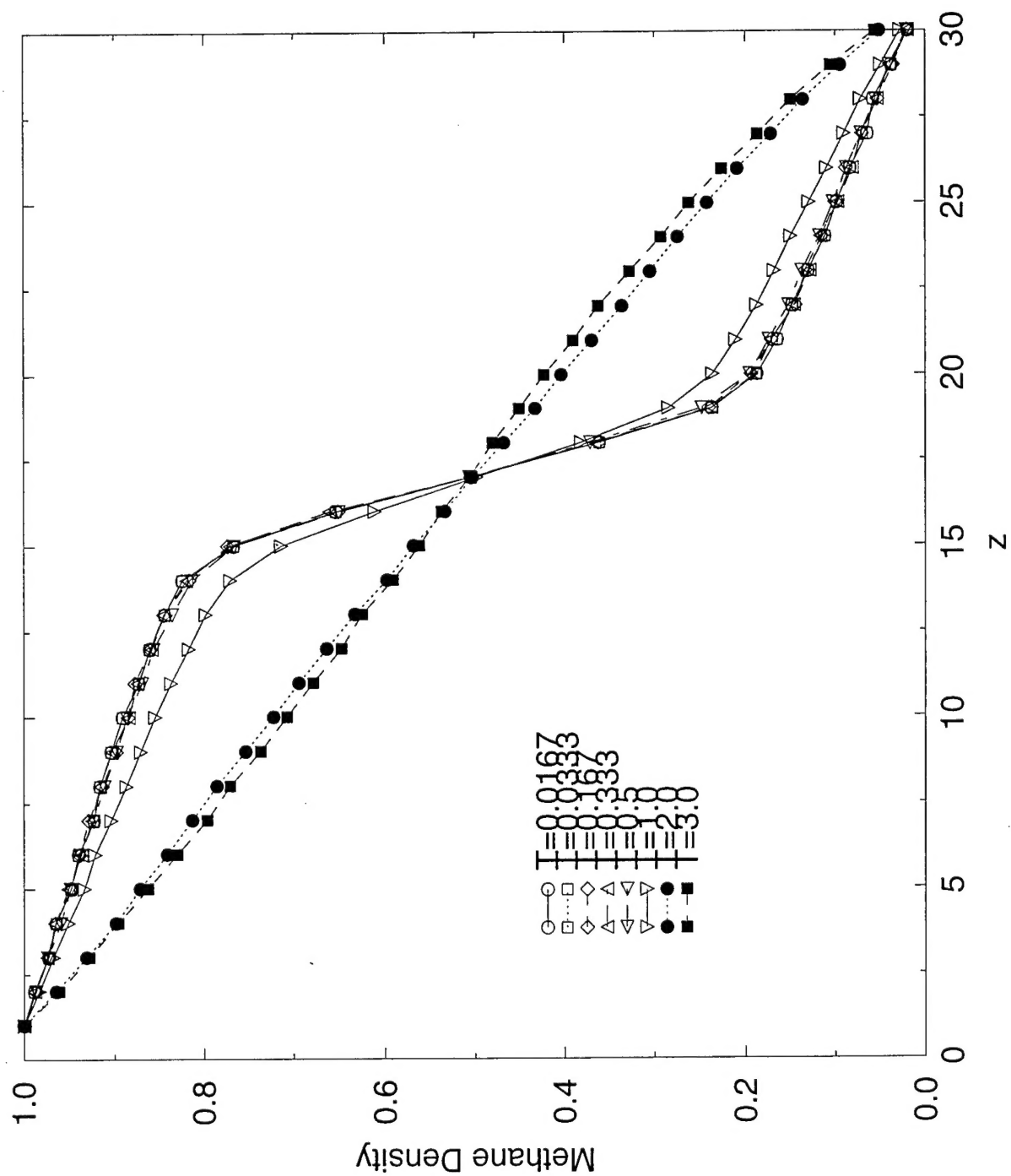


Figure 3(b)

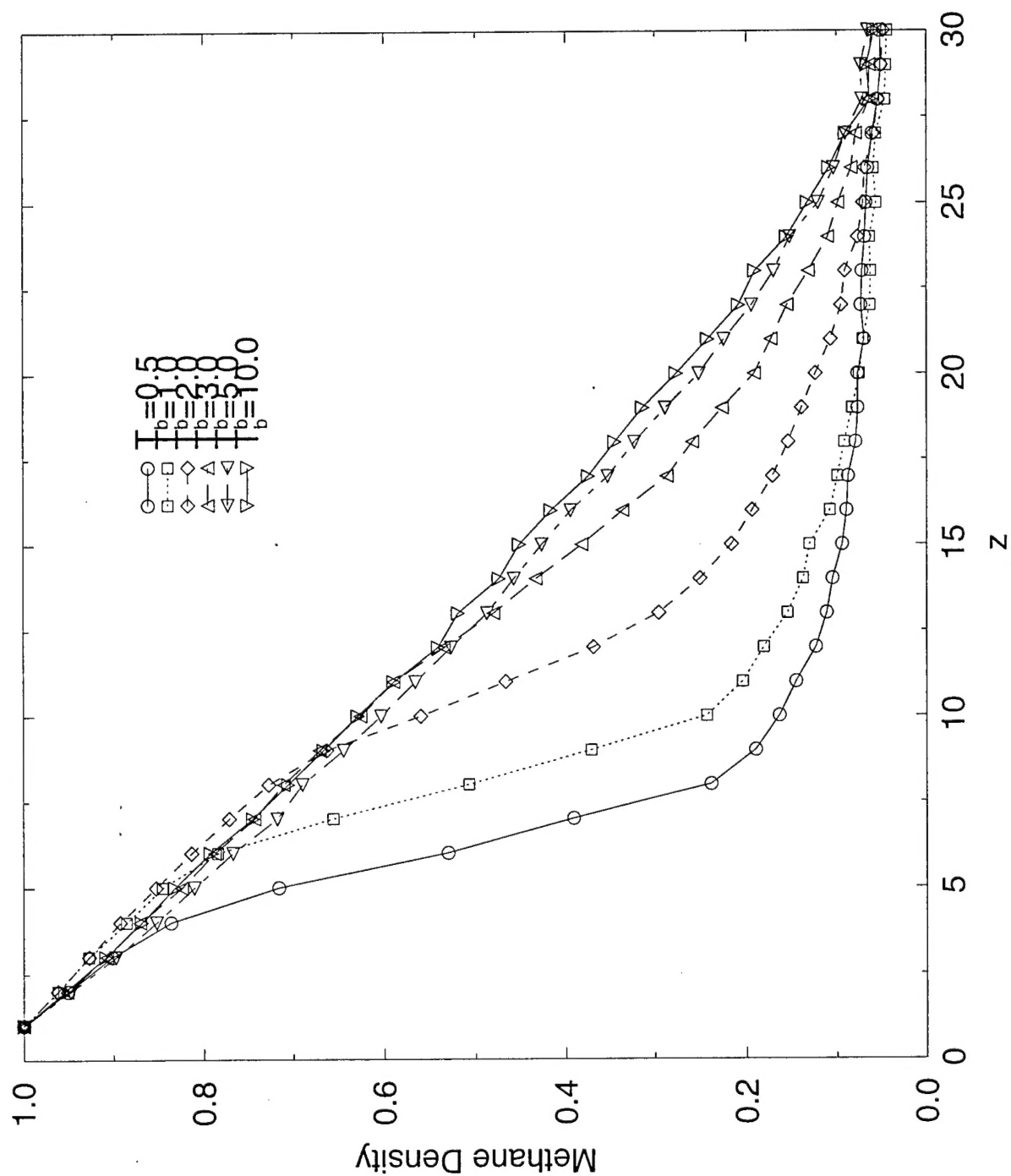


Figure 4

